



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:31 AM UTC

PDB ID : 1DUW / pdb_00001duw
Title : STRUCTURE OF NONAHEME CYTOCHROME C
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Deposited on : 2000-01-19
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

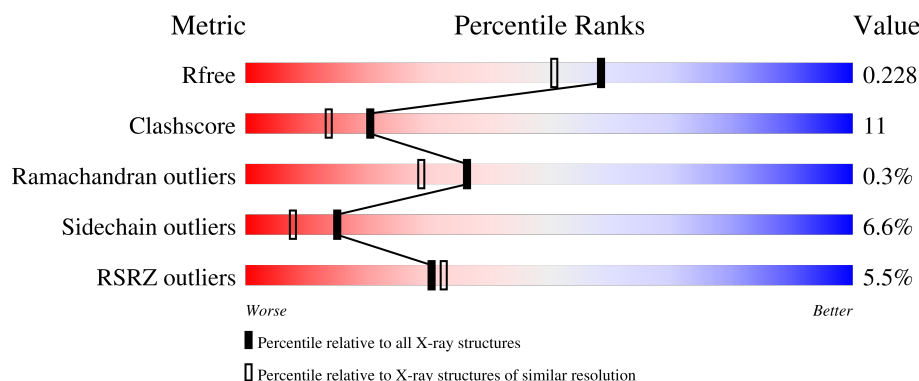
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	292	5% 72% 23% ...

2 Entry composition i

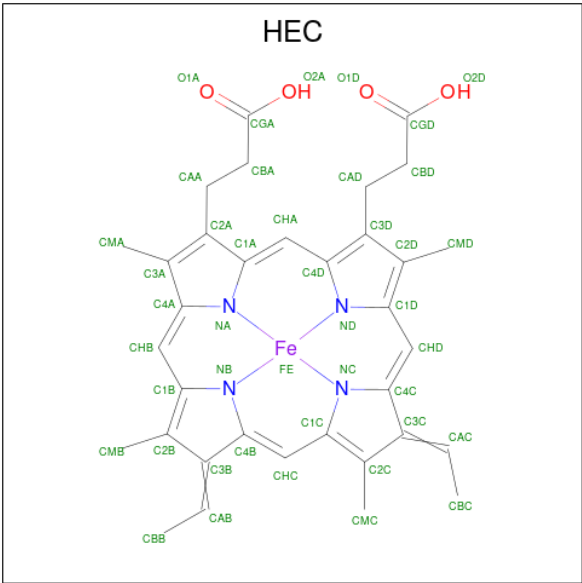
There are 4 unique types of molecules in this entry. The entry contains 3004 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NONAHEME CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2188	1334	415	411	28			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



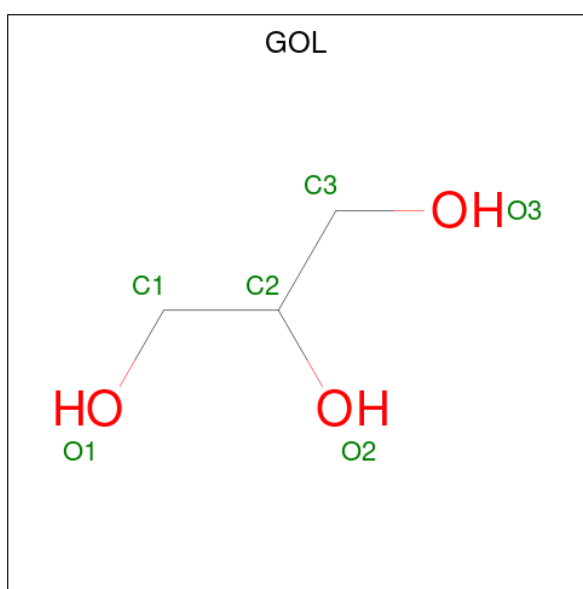
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

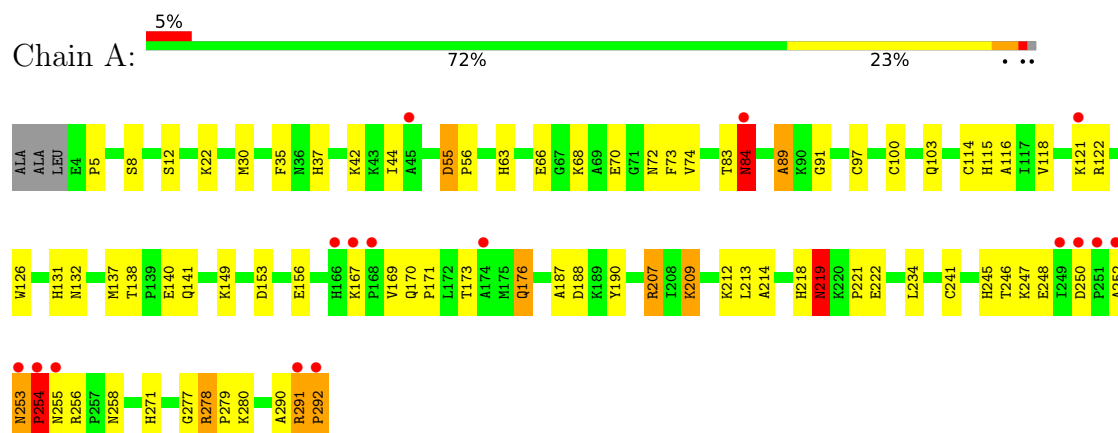
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	423	Total	O	0	0
			423	423		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NONAHEME CYTOCHROME C



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	55.40Å 55.40Å 236.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.89 30.00 – 1.89	Depositor EDS
% Data completeness (in resolution range)	7.5 (30.00-1.89) 98.5 (30.00-1.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.88Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.183 , 0.235 0.182 , 0.228	Depositor DCC
R_{free} test set	2143 reflections (6.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3004	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.79	1/2246 (0.0%)	1.62	27/3044 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	PRO	C-OXT	81.08	2.85	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CA-CB-CG	12.34	124.94	112.60
1	A	115	HIS	CA-CB-CG	-9.90	103.90	113.80
1	A	253	ASN	CA-CB-CG	8.61	121.20	112.60
1	A	84	ASN	CA-CB-CG	8.52	121.12	112.60
1	A	254	PRO	CA-N-CD	-6.84	101.92	111.50
1	A	73	PHE	CA-CB-CG	-6.81	106.99	113.80
1	A	153	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	207	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	A	271	HIS	CA-C-O	6.16	127.50	120.90
1	A	91	GLY	CA-C-N	6.15	130.22	121.42
1	A	91	GLY	C-N-CA	6.15	130.22	121.42
1	A	131	HIS	CA-CB-CG	-6.08	107.72	113.80
1	A	132	ASN	N-CA-C	5.84	120.24	112.30
1	A	37	HIS	CA-CB-CG	-5.68	108.11	113.80
1	A	219	ASN	N-CA-C	5.68	119.20	112.72
1	A	207	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	254	PRO	CA-C-N	5.51	132.33	121.58
1	A	254	PRO	C-N-CA	5.51	132.33	121.58
1	A	89	ALA	CA-C-N	-5.46	113.63	122.81
1	A	89	ALA	C-N-CA	-5.46	113.63	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	250	ASP	CB-CA-C	5.35	115.89	109.31
1	A	132	ASN	N-CA-CB	-5.33	102.64	111.49
1	A	247	LYS	CA-C-O	5.29	126.34	120.63
1	A	83	THR	CA-C-O	-5.24	115.50	121.68
1	A	250	ASP	CA-C-O	5.10	125.32	119.61
1	A	116	ALA	N-CA-C	-5.08	106.59	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2188	0	2124	53	0
2	A	387	0	270	10	0
3	A	6	0	8	0	0
4	A	423	0	0	13	0
All	All	3004	0	2402	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PRO:HD2	1:A:256:ARG:H	1.39	0.87
1:A:173:THR:H	1:A:176:GLN:HE21	1.25	0.83
1:A:138:THR:H	1:A:141:GLN:HE21	1.29	0.77
1:A:56:PRO:HG3	4:A:1279:HOH:O	1.85	0.76
1:A:169:VAL:HG21	1:A:219:ASN:O	1.86	0.75
1:A:173:THR:H	1:A:176:GLN:NE2	1.86	0.74
1:A:254:PRO:HD3	4:A:1407:HOH:O	1.87	0.73
1:A:277:GLY:O	1:A:280:LYS:HE3	1.89	0.73
1:A:255:ASN:HA	4:A:1336:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ARG:HD2	4:A:1045:HOH:O	1.93	0.68
1:A:22:LYS:HG3	1:A:66:GLU:OE2	1.93	0.67
1:A:68:LYS:HG3	1:A:70:GLU:OE1	1.99	0.62
1:A:89:ALA:HB2	4:A:1232:HOH:O	2.01	0.61
2:A:297:HEC:HMC1	2:A:297:HEC:HBC3	1.82	0.60
2:A:298:HEC:HMC1	2:A:298:HEC:HBC3	1.85	0.56
1:A:140:GLU:HB2	4:A:1355:HOH:O	2.05	0.56
1:A:246:THR:O	1:A:258:ASN:HB2	2.10	0.52
1:A:209:LYS:NZ	1:A:209:LYS:HB3	2.25	0.52
1:A:171:PRO:HA	1:A:221:PRO:HA	1.92	0.51
1:A:188:ASP:O	1:A:291:ARG:HD3	2.11	0.51
1:A:140:GLU:HA	1:A:140:GLU:OE1	2.10	0.51
1:A:8:SER:HB2	2:A:296:HEC:C2B	2.41	0.50
1:A:138:THR:H	1:A:141:GLN:NE2	2.05	0.50
1:A:291:ARG:O	1:A:292:PRO:O	2.30	0.49
1:A:254:PRO:HD2	1:A:256:ARG:HB2	1.94	0.49
1:A:213:LEU:HD13	2:A:297:HEC:CHA	2.43	0.49
1:A:207:ARG:HG3	4:A:1322:HOH:O	2.12	0.48
1:A:241:CYS:HA	2:A:298:HEC:HHC	1.95	0.48
1:A:35:PHE:CZ	2:A:296:HEC:HHD	2.49	0.48
1:A:190:TYR:CD2	1:A:290:ALA:HA	2.49	0.47
1:A:30:MET:HG3	2:A:294:HEC:C4A	2.45	0.47
1:A:187:ALA:HB3	4:A:1176:HOH:O	2.15	0.47
1:A:63:HIS:CE1	1:A:74:VAL:HB	2.50	0.46
1:A:207:ARG:NH2	4:A:1322:HOH:O	2.48	0.46
1:A:122:ARG:HD3	1:A:126:TRP:CH2	2.51	0.46
1:A:254:PRO:CD	1:A:256:ARG:HB2	2.46	0.45
1:A:5:PRO:HA	4:A:1301:HOH:O	2.16	0.45
1:A:114:CYS:O	1:A:118:VAL:HG23	2.17	0.45
1:A:138:THR:OG1	1:A:141:GLN:HG3	2.16	0.45
1:A:84:ASN:O	1:A:84:ASN:ND2	2.50	0.45
1:A:188:ASP:O	1:A:291:ARG:NH1	2.49	0.44
1:A:214:ALA:HB1	1:A:218:HIS:CE1	2.53	0.44
1:A:212:LYS:HD3	4:A:1058:HOH:O	2.17	0.44
1:A:241:CYS:HA	2:A:298:HEC:CHC	2.47	0.44
2:A:296:HEC:HMC1	2:A:296:HEC:HBC3	1.99	0.44
1:A:100:CYS:O	1:A:103:GLN:HB2	2.18	0.43
1:A:156:GLU:HA	4:A:1152:HOH:O	2.18	0.43
1:A:252:ALA:O	1:A:254:PRO:HA	2.18	0.43
1:A:248:GLU:HA	1:A:248:GLU:OE1	2.19	0.43
1:A:55:ASP:HA	1:A:56:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HG2	1:A:279:PRO:N	2.26	0.41
1:A:137:MET:HA	1:A:141:GLN:NE2	2.35	0.41
1:A:222:GLU:HB2	1:A:234:LEU:HD13	2.03	0.41
1:A:97:CYS:HA	2:A:297:HEC:CHC	2.51	0.41
1:A:280:LYS:HA	1:A:280:LYS:HD3	1.91	0.40
1:A:248:GLU:HB2	4:A:1142:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	288/292 (99%)	279 (97%)	8 (3%)	1 (0%)	36 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	242/242 (100%)	226 (93%)	16 (7%)	15 8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	42	LYS
1	A	44	ILE
1	A	55	ASP
1	A	72	ASN
1	A	84	ASN
1	A	121	LYS
1	A	149	LYS
1	A	167	LYS
1	A	170	GLN
1	A	176	GLN
1	A	209	LYS
1	A	219	ASN
1	A	253	ASN
1	A	278	ARG
1	A	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	141	GLN
1	A	143	GLN
1	A	154	GLN
1	A	165	ASN
1	A	176	GLN
1	A	194	ASN
1	A	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	299	1	46,50,50	1.33	2 (4%)	58,82,82	2.26	14 (24%)
2	HEC	A	295	1	46,50,50	1.37	2 (4%)	58,82,82	2.17	18 (31%)
2	HEC	A	293	1	46,50,50	1.35	2 (4%)	58,82,82	2.14	18 (31%)
2	HEC	A	296	1	46,50,50	1.34	2 (4%)	58,82,82	2.40	19 (32%)
2	HEC	A	300	1	46,50,50	1.32	2 (4%)	58,82,82	2.28	18 (31%)
2	HEC	A	301	1	46,50,50	1.34	2 (4%)	58,82,82	2.33	18 (31%)
2	HEC	A	294	1	46,50,50	1.32	2 (4%)	58,82,82	2.16	16 (27%)
2	HEC	A	298	1	46,50,50	1.34	2 (4%)	58,82,82	2.28	14 (24%)
3	GOL	A	302	-	5,5,5	0.79	0	5,5,5	0.70	0
2	HEC	A	297	1	46,50,50	1.32	2 (4%)	58,82,82	2.14	17 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	299	1	-	4/14/54/54	-
2	HEC	A	295	1	-	8/14/54/54	-
2	HEC	A	293	1	-	4/14/54/54	-
2	HEC	A	296	1	-	8/14/54/54	-
2	HEC	A	300	1	-	5/14/54/54	-
2	HEC	A	301	1	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	294	1	-	8/14/54/54	-
2	HEC	A	298	1	-	6/14/54/54	-
3	GOL	A	302	-	-	0/4/4/4	-
2	HEC	A	297	1	-	8/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	296	HEC	CAB-C3B	5.46	1.52	1.35
2	A	299	HEC	CAC-C3C	5.43	1.52	1.35
2	A	295	HEC	CAB-C3B	5.42	1.52	1.35
2	A	301	HEC	CAB-C3B	5.34	1.52	1.35
2	A	299	HEC	CAB-C3B	5.29	1.52	1.35
2	A	297	HEC	CAB-C3B	5.29	1.52	1.35
2	A	298	HEC	CAB-C3B	5.24	1.52	1.35
2	A	298	HEC	CAC-C3C	5.23	1.52	1.35
2	A	300	HEC	CAB-C3B	5.22	1.52	1.35
2	A	294	HEC	CAC-C3C	5.15	1.51	1.35
2	A	295	HEC	CAC-C3C	5.15	1.51	1.35
2	A	296	HEC	CAC-C3C	5.14	1.51	1.35
2	A	301	HEC	CAC-C3C	5.14	1.51	1.35
2	A	293	HEC	CAC-C3C	5.13	1.51	1.35
2	A	293	HEC	CAB-C3B	5.09	1.51	1.35
2	A	294	HEC	CAB-C3B	5.03	1.51	1.35
2	A	300	HEC	CAC-C3C	5.01	1.51	1.35
2	A	297	HEC	CAC-C3C	4.80	1.50	1.35

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	HEC	CBB-CAB-C3B	-8.46	110.52	127.43
2	A	298	HEC	CBC-CAC-C3C	-7.78	111.89	127.43
2	A	296	HEC	CBB-CAB-C3B	-7.68	112.07	127.43
2	A	299	HEC	CBC-CAC-C3C	-7.51	112.43	127.43
2	A	295	HEC	CBC-CAC-C3C	-7.44	112.57	127.43
2	A	300	HEC	CBC-CAC-C3C	-6.83	113.79	127.43
2	A	301	HEC	CBB-CAB-C3B	-6.79	113.86	127.43
2	A	294	HEC	CBB-CAB-C3B	-6.77	113.89	127.43
2	A	297	HEC	CBB-CAB-C3B	-6.71	114.03	127.43
2	A	298	HEC	CBB-CAB-C3B	-6.58	114.29	127.43
2	A	293	HEC	CBC-CAC-C3C	-6.43	114.58	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	HEC	CBB-CAB-C3B	-6.32	114.81	127.43
2	A	300	HEC	CBB-CAB-C3B	-6.11	115.23	127.43
2	A	300	HEC	CHA-C1A-NA	5.87	130.84	124.45
2	A	294	HEC	CBC-CAC-C3C	-5.74	115.97	127.43
2	A	293	HEC	CBB-CAB-C3B	-5.72	116.00	127.43
2	A	296	HEC	CBC-CAC-C3C	-5.62	116.20	127.43
2	A	301	HEC	CBC-CAC-C3C	-5.54	116.36	127.43
2	A	298	HEC	CHC-C4B-NB	5.29	130.21	124.45
2	A	301	HEC	CHC-C4B-NB	5.26	130.18	124.45
2	A	296	HEC	CHA-C1A-NA	5.18	130.09	124.45
2	A	296	HEC	C3D-C4D-ND	-5.15	104.43	110.15
2	A	296	HEC	CHB-C4A-NA	5.09	130.00	124.45
2	A	301	HEC	CHA-C1A-NA	4.94	129.83	124.45
2	A	297	HEC	CHC-C4B-NB	4.65	129.51	124.45
2	A	293	HEC	CHB-C4A-NA	4.60	129.46	124.45
2	A	299	HEC	CHB-C4A-NA	4.59	129.46	124.45
2	A	300	HEC	CHB-C4A-NA	4.58	129.44	124.45
2	A	298	HEC	CHB-C4A-NA	4.48	129.33	124.45
2	A	296	HEC	C2A-C1A-NA	-4.36	106.11	110.32
2	A	295	HEC	CHB-C4A-NA	4.33	129.17	124.45
2	A	300	HEC	CHD-C4C-NC	4.31	129.14	124.45
2	A	296	HEC	CHC-C4B-NB	4.30	129.14	124.45
2	A	297	HEC	CHB-C4A-NA	4.29	129.12	124.45
2	A	293	HEC	CHD-C4C-NC	4.18	129.00	124.45
2	A	297	HEC	CBC-CAC-C3C	-4.15	119.13	127.43
2	A	295	HEC	CHC-C4B-NB	4.14	128.96	124.45
2	A	299	HEC	CHA-C1A-NA	4.12	128.94	124.45
2	A	301	HEC	CHB-C4A-NA	4.12	128.94	124.45
2	A	294	HEC	CHC-C1C-NC	4.11	131.32	123.86
2	A	297	HEC	CHA-C1A-NA	4.11	128.93	124.45
2	A	301	HEC	CMC-C2C-C1C	-4.07	119.22	125.42
2	A	294	HEC	CHB-C4A-NA	3.94	128.75	124.45
2	A	298	HEC	CHA-C1A-NA	3.94	128.74	124.45
2	A	295	HEC	CHC-C1C-NC	3.93	130.99	123.86
2	A	294	HEC	CMC-C2C-C1C	-3.93	119.43	125.42
2	A	299	HEC	CHC-C4B-NB	3.74	128.53	124.45
2	A	300	HEC	C2A-C1A-NA	-3.69	106.76	110.32
2	A	295	HEC	CHB-C1B-NB	3.68	130.54	123.86
2	A	299	HEC	CHD-C4C-NC	3.62	128.40	124.45
2	A	293	HEC	CHA-C1A-NA	3.60	128.37	124.45
2	A	293	HEC	CHD-C1D-ND	3.53	130.26	123.86
2	A	294	HEC	CHA-C1A-NA	3.50	128.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	HEC	CHA-C1A-NA	3.48	128.24	124.45
2	A	297	HEC	C3D-C4D-ND	-3.46	106.31	110.15
2	A	301	HEC	CHD-C1D-ND	3.41	130.05	123.86
2	A	301	HEC	C2A-C1A-NA	-3.39	107.06	110.32
2	A	298	HEC	CHC-C1C-NC	3.39	130.00	123.86
2	A	301	HEC	CHC-C1C-NC	3.38	129.99	123.86
2	A	297	HEC	C2A-C1A-NA	-3.38	107.06	110.32
2	A	294	HEC	CHC-C4B-NB	3.38	128.13	124.45
2	A	297	HEC	CHC-C1C-NC	3.36	129.96	123.86
2	A	298	HEC	CHB-C1B-NB	3.36	129.96	123.86
2	A	301	HEC	CMD-C2D-C1D	-3.35	120.31	125.42
2	A	296	HEC	CHD-C4C-C3C	-3.33	119.60	125.21
2	A	294	HEC	CHB-C1B-NB	3.28	129.81	123.86
2	A	293	HEC	CHC-C1C-NC	3.19	129.65	123.86
2	A	301	HEC	CHB-C1B-NB	3.17	129.62	123.86
2	A	293	HEC	C3D-C4D-ND	-3.17	106.63	110.15
2	A	297	HEC	CHB-C1B-NB	3.16	129.59	123.86
2	A	293	HEC	C2A-C1A-NA	-3.11	107.32	110.32
2	A	297	HEC	CHD-C1D-ND	3.11	129.51	123.86
2	A	300	HEC	CHC-C1C-NC	3.08	129.44	123.86
2	A	294	HEC	C2D-C1D-ND	-3.07	105.22	110.14
2	A	296	HEC	C4A-NA-C1A	3.03	110.76	105.82
2	A	300	HEC	C4C-NC-C1C	3.01	110.73	105.82
2	A	298	HEC	C3D-C4D-ND	-2.99	106.84	110.15
2	A	294	HEC	C3D-C4D-ND	-2.97	106.86	110.15
2	A	300	HEC	CHB-C1B-NB	2.96	129.22	123.86
2	A	295	HEC	CMC-C2C-C1C	-2.90	121.01	125.42
2	A	294	HEC	C2A-C1A-NA	-2.86	107.57	110.32
2	A	298	HEC	C2A-C1A-NA	-2.85	107.58	110.32
2	A	301	HEC	CHD-C4C-NC	2.82	127.52	124.45
2	A	299	HEC	CHB-C1B-NB	2.82	128.97	123.86
2	A	293	HEC	CHC-C4B-NB	2.81	127.52	124.45
2	A	299	HEC	CHA-C4D-ND	2.79	128.92	123.86
2	A	296	HEC	CHB-C1B-NB	2.77	128.89	123.86
2	A	299	HEC	C3D-C4D-ND	-2.74	107.11	110.15
2	A	299	HEC	CHC-C1C-NC	2.73	128.81	123.86
2	A	301	HEC	C3D-C4D-ND	-2.72	107.14	110.15
2	A	300	HEC	C4A-NA-C1A	2.67	110.17	105.82
2	A	299	HEC	C2A-C1A-NA	-2.66	107.75	110.32
2	A	297	HEC	CMC-C2C-C1C	-2.65	121.38	125.42
2	A	297	HEC	C4A-NA-C1A	2.63	110.12	105.82
2	A	300	HEC	CAA-C2A-C1A	-2.62	119.53	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	296	HEC	O1D-CGD-CBD	-2.58	114.92	123.09
2	A	293	HEC	C4A-NA-C1A	2.54	109.97	105.82
2	A	294	HEC	C4C-NC-C1C	2.54	109.97	105.82
2	A	300	HEC	O1A-CGA-CBA	-2.51	115.12	123.09
2	A	293	HEC	C4D-ND-C1D	2.51	109.91	105.82
2	A	296	HEC	CHD-C1D-C2D	-2.49	120.21	127.43
2	A	294	HEC	CMB-C2B-C1B	-2.46	121.67	125.42
2	A	300	HEC	C2C-C1C-NC	-2.44	106.24	110.14
2	A	296	HEC	CMD-C2D-C3D	2.43	130.78	125.62
2	A	301	HEC	CMC-C2C-C3C	2.43	132.26	126.55
2	A	293	HEC	CHB-C1B-NB	2.41	128.23	123.86
2	A	295	HEC	C2A-C1A-NA	-2.41	108.00	110.32
2	A	296	HEC	CMD-C2D-C1D	-2.39	121.78	125.42
2	A	300	HEC	CHC-C4B-NB	2.38	127.05	124.45
2	A	297	HEC	C4B-NB-C1B	2.38	109.70	105.82
2	A	296	HEC	O1A-CGA-CBA	-2.37	115.58	123.09
2	A	296	HEC	CHC-C1C-NC	2.34	128.11	123.86
2	A	295	HEC	CHD-C4C-NC	2.34	127.00	124.45
2	A	301	HEC	C4A-NA-C1A	2.31	109.59	105.82
2	A	298	HEC	C4B-NB-C1B	2.31	109.59	105.82
2	A	293	HEC	C4C-NC-C1C	2.30	109.58	105.82
2	A	301	HEC	C4D-ND-C1D	2.30	109.56	105.82
2	A	298	HEC	CMB-C2B-C1B	-2.29	121.92	125.42
2	A	293	HEC	CHD-C4C-C3C	-2.28	121.36	125.21
2	A	295	HEC	C3D-C4D-ND	-2.28	107.62	110.15
2	A	296	HEC	C1D-CHD-C4C	-2.27	117.66	124.66
2	A	300	HEC	CHD-C1D-C2D	-2.26	120.87	127.43
2	A	294	HEC	CHD-C1D-C2D	-2.25	120.89	127.43
2	A	298	HEC	C4C-NC-C1C	2.24	109.47	105.82
2	A	293	HEC	CHA-C4D-ND	2.20	127.86	123.86
2	A	300	HEC	CHA-C4D-ND	2.20	127.85	123.86
2	A	295	HEC	CHC-C1C-C2C	-2.20	121.04	127.43
2	A	297	HEC	CHD-C4C-C3C	-2.19	121.51	125.21
2	A	299	HEC	C4A-NA-C1A	2.17	109.37	105.82
2	A	295	HEC	CMB-C2B-C1B	-2.17	122.11	125.42
2	A	293	HEC	O1D-CGD-CBD	-2.17	116.20	123.09
2	A	296	HEC	C2D-C1D-ND	-2.17	106.66	110.14
2	A	295	HEC	CHD-C1D-ND	2.17	127.79	123.86
2	A	298	HEC	C2D-C1D-ND	-2.15	106.70	110.14
2	A	297	HEC	C4D-ND-C1D	2.15	109.32	105.82
2	A	295	HEC	C4A-NA-C1A	2.14	109.31	105.82
2	A	301	HEC	C4B-NB-C1B	2.11	109.27	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	296	HEC	CAA-C2A-C1A	-2.10	120.58	124.85
2	A	299	HEC	CHD-C1D-ND	2.08	127.64	123.86
2	A	298	HEC	C4A-NA-C1A	2.08	109.22	105.82
2	A	294	HEC	C4A-NA-C1A	2.08	109.21	105.82
2	A	299	HEC	C4C-NC-C1C	2.08	109.20	105.82
2	A	295	HEC	C4C-NC-C1C	2.06	109.18	105.82
2	A	300	HEC	C3D-C4D-ND	-2.06	107.87	110.15
2	A	300	HEC	C4D-ND-C1D	2.05	109.16	105.82
2	A	295	HEC	CHB-C1B-C2B	-2.03	121.52	127.43
2	A	294	HEC	CHA-C4D-ND	2.03	127.55	123.86
2	A	297	HEC	O1D-CGD-CBD	-2.02	116.69	123.09
2	A	301	HEC	CHA-C4D-ND	2.00	127.49	123.86
2	A	297	HEC	CHD-C4C-NC	2.00	126.64	124.45
2	A	293	HEC	CMD-C2D-C3D	2.00	129.87	125.62
2	A	295	HEC	CHA-C4D-ND	2.00	127.49	123.86

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	293	HEC	C2B-C3B-CAB-CBB
2	A	293	HEC	C4B-C3B-CAB-CBB
2	A	293	HEC	C2C-C3C-CAC-CBC
2	A	293	HEC	C4C-C3C-CAC-CBC
2	A	294	HEC	C2B-C3B-CAB-CBB
2	A	294	HEC	C4B-C3B-CAB-CBB
2	A	294	HEC	C2C-C3C-CAC-CBC
2	A	294	HEC	C4C-C3C-CAC-CBC
2	A	295	HEC	C2B-C3B-CAB-CBB
2	A	295	HEC	C4B-C3B-CAB-CBB
2	A	295	HEC	C2C-C3C-CAC-CBC
2	A	295	HEC	C4C-C3C-CAC-CBC
2	A	296	HEC	C2B-C3B-CAB-CBB
2	A	296	HEC	C4B-C3B-CAB-CBB
2	A	296	HEC	C2C-C3C-CAC-CBC
2	A	296	HEC	C4C-C3C-CAC-CBC
2	A	297	HEC	C2A-CAA-CBA-CGA
2	A	297	HEC	C2B-C3B-CAB-CBB
2	A	297	HEC	C4B-C3B-CAB-CBB
2	A	297	HEC	C2C-C3C-CAC-CBC
2	A	297	HEC	C4C-C3C-CAC-CBC
2	A	298	HEC	C2B-C3B-CAB-CBB

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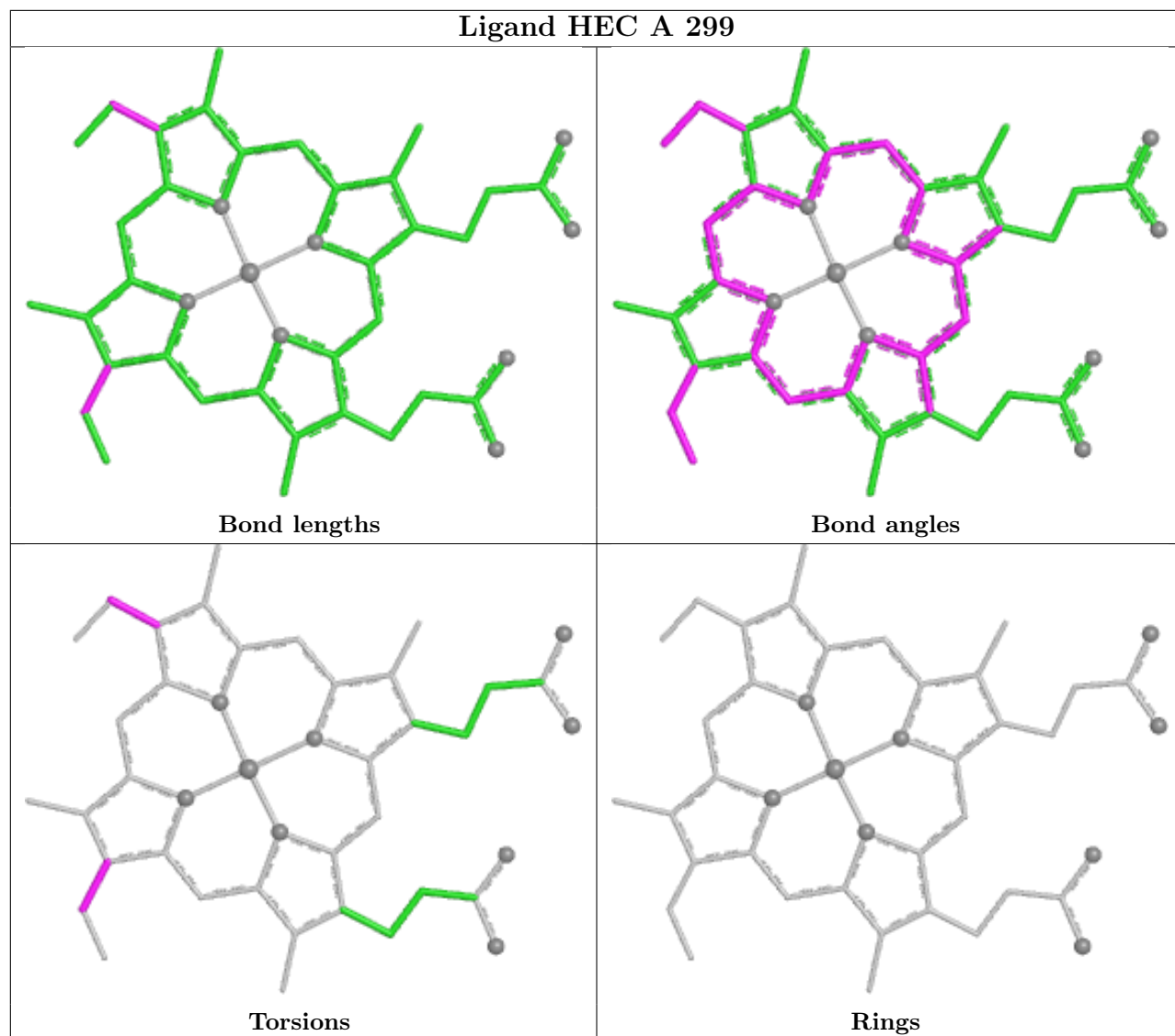
Mol	Chain	Res	Type	Atoms
2	A	298	HEC	C4B-C3B-CAB-CBB
2	A	298	HEC	C2C-C3C-CAC-CBC
2	A	298	HEC	C4C-C3C-CAC-CBC
2	A	299	HEC	C2B-C3B-CAB-CBB
2	A	299	HEC	C4B-C3B-CAB-CBB
2	A	299	HEC	C2C-C3C-CAC-CBC
2	A	299	HEC	C4C-C3C-CAC-CBC
2	A	300	HEC	C2B-C3B-CAB-CBB
2	A	300	HEC	C4B-C3B-CAB-CBB
2	A	300	HEC	C2C-C3C-CAC-CBC
2	A	300	HEC	C4C-C3C-CAC-CBC
2	A	301	HEC	C2B-C3B-CAB-CBB
2	A	301	HEC	C4B-C3B-CAB-CBB
2	A	301	HEC	C2C-C3C-CAC-CBC
2	A	301	HEC	C4C-C3C-CAC-CBC
2	A	301	HEC	C2A-CAA-CBA-CGA
2	A	294	HEC	CAD-CBD-CGD-O2D
2	A	294	HEC	CAD-CBD-CGD-O1D
2	A	301	HEC	CAD-CBD-CGD-O2D
2	A	296	HEC	CAA-CBA-CGA-O2A
2	A	301	HEC	CAD-CBD-CGD-O1D
2	A	294	HEC	CAA-CBA-CGA-O2A
2	A	298	HEC	CAA-CBA-CGA-O1A
2	A	294	HEC	CAA-CBA-CGA-O1A
2	A	297	HEC	CAA-CBA-CGA-O2A
2	A	295	HEC	CAA-CBA-CGA-O2A
2	A	296	HEC	CAA-CBA-CGA-O1A
2	A	296	HEC	CAD-CBD-CGD-O2D
2	A	298	HEC	CAA-CBA-CGA-O2A
2	A	297	HEC	CAD-CBD-CGD-O2D
2	A	295	HEC	CAA-CBA-CGA-O1A
2	A	295	HEC	CAD-CBD-CGD-O1D
2	A	297	HEC	CAA-CBA-CGA-O1A
2	A	296	HEC	CAD-CBD-CGD-O1D
2	A	295	HEC	CAD-CBD-CGD-O2D
2	A	301	HEC	CAA-CBA-CGA-O1A
2	A	300	HEC	CAD-CBD-CGD-O1D

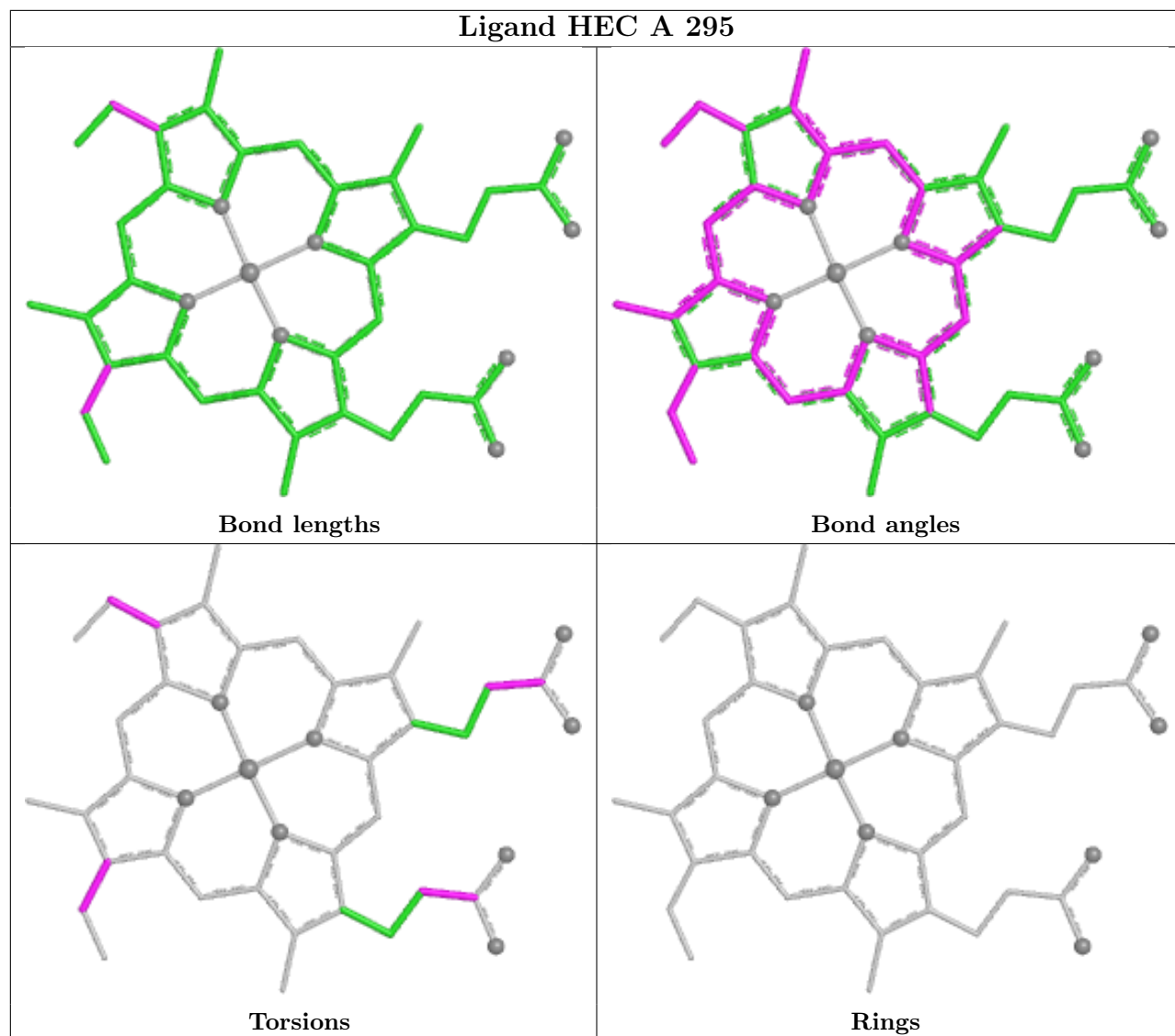
There are no ring outliers.

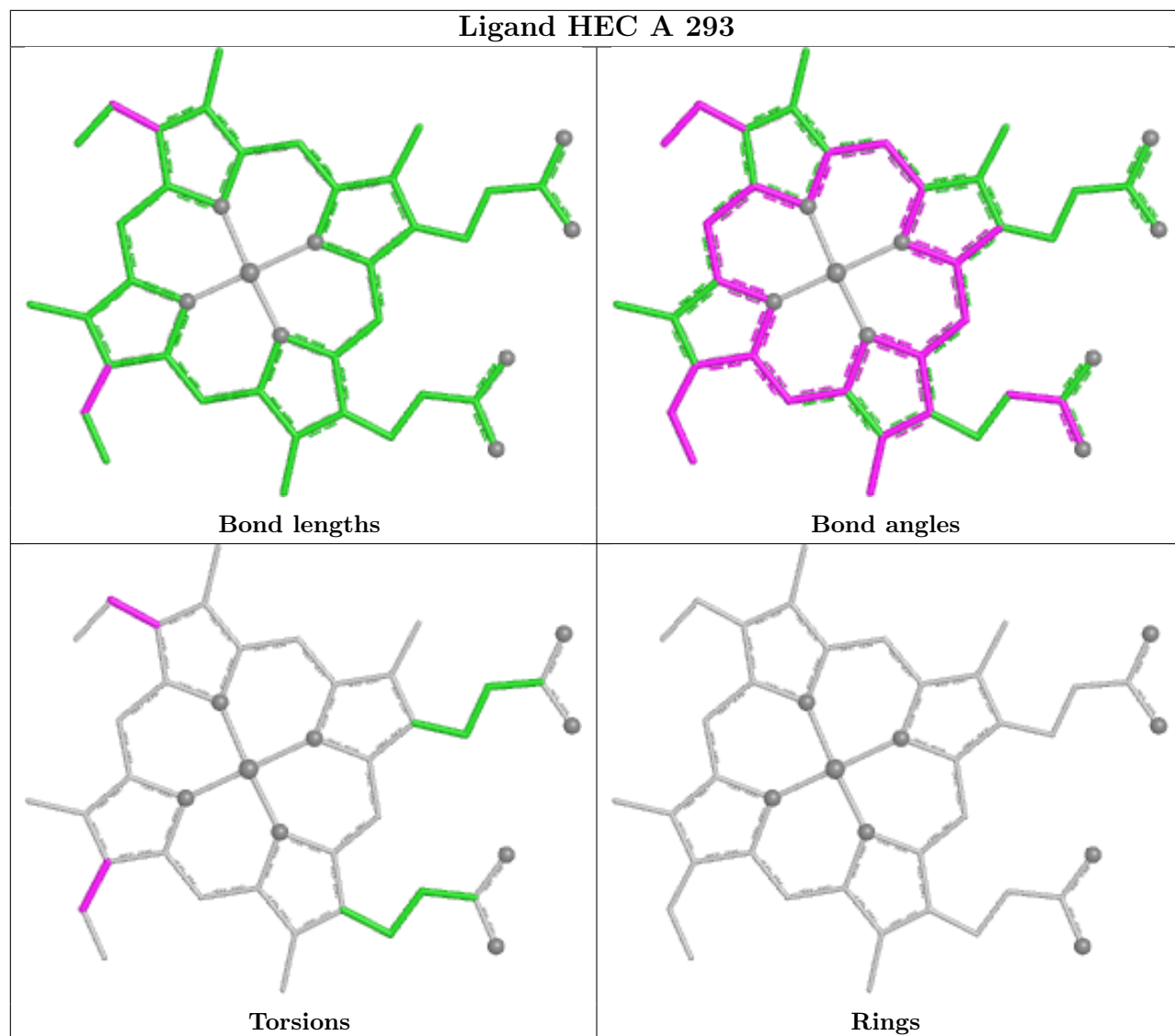
4 monomers are involved in 10 short contacts:

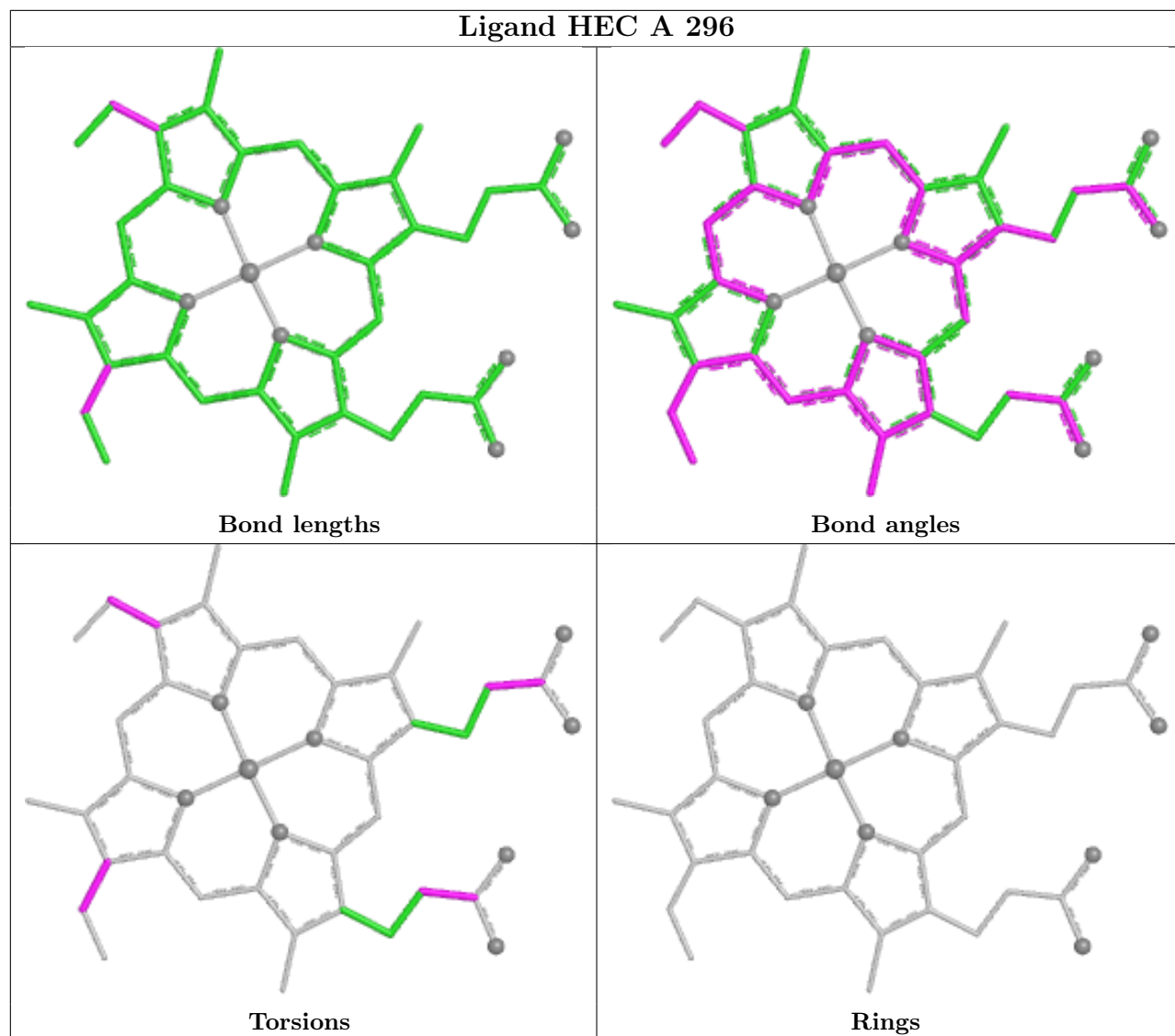
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	296	HEC	3	0
2	A	294	HEC	1	0
2	A	298	HEC	3	0
2	A	297	HEC	3	0

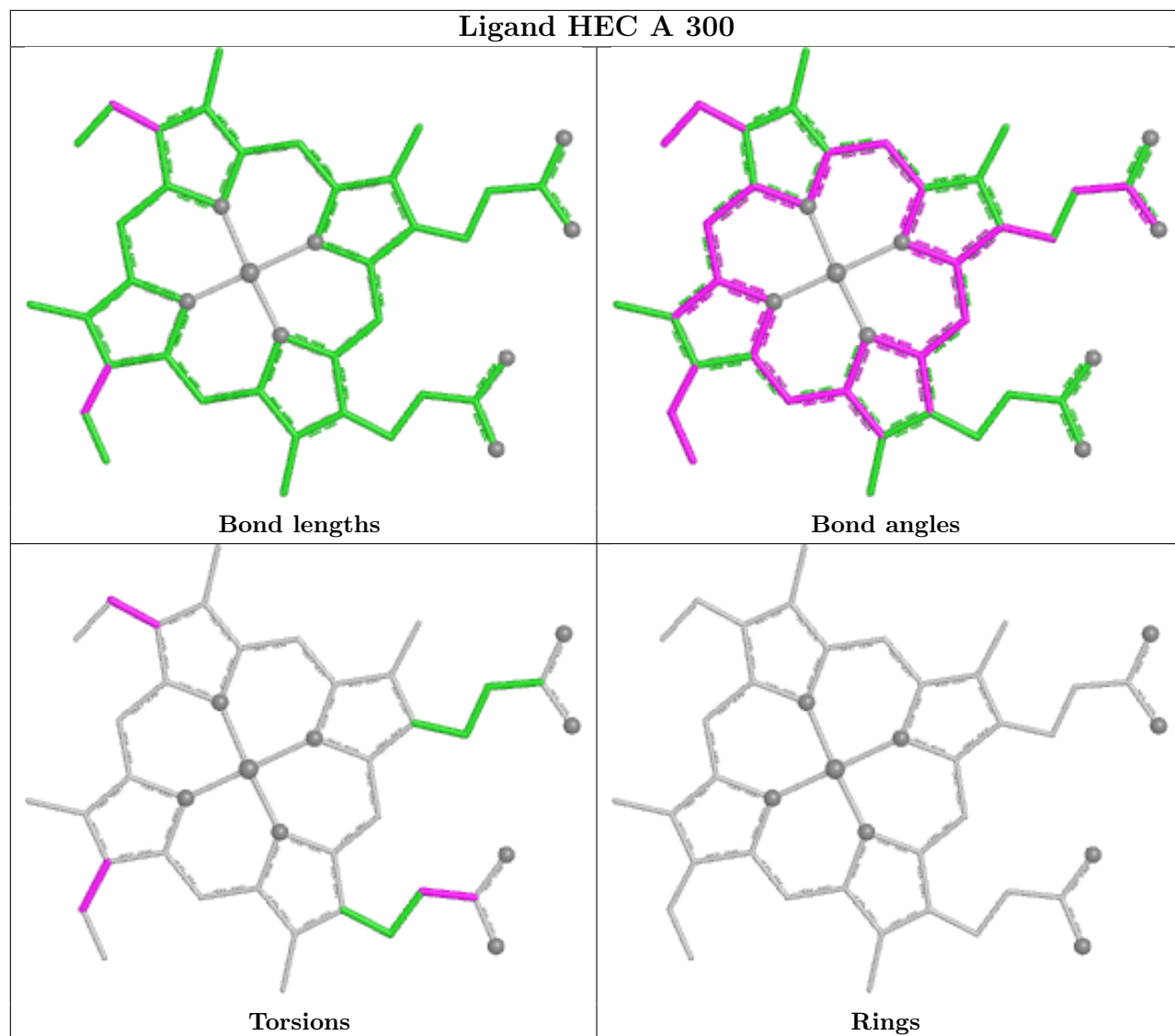
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

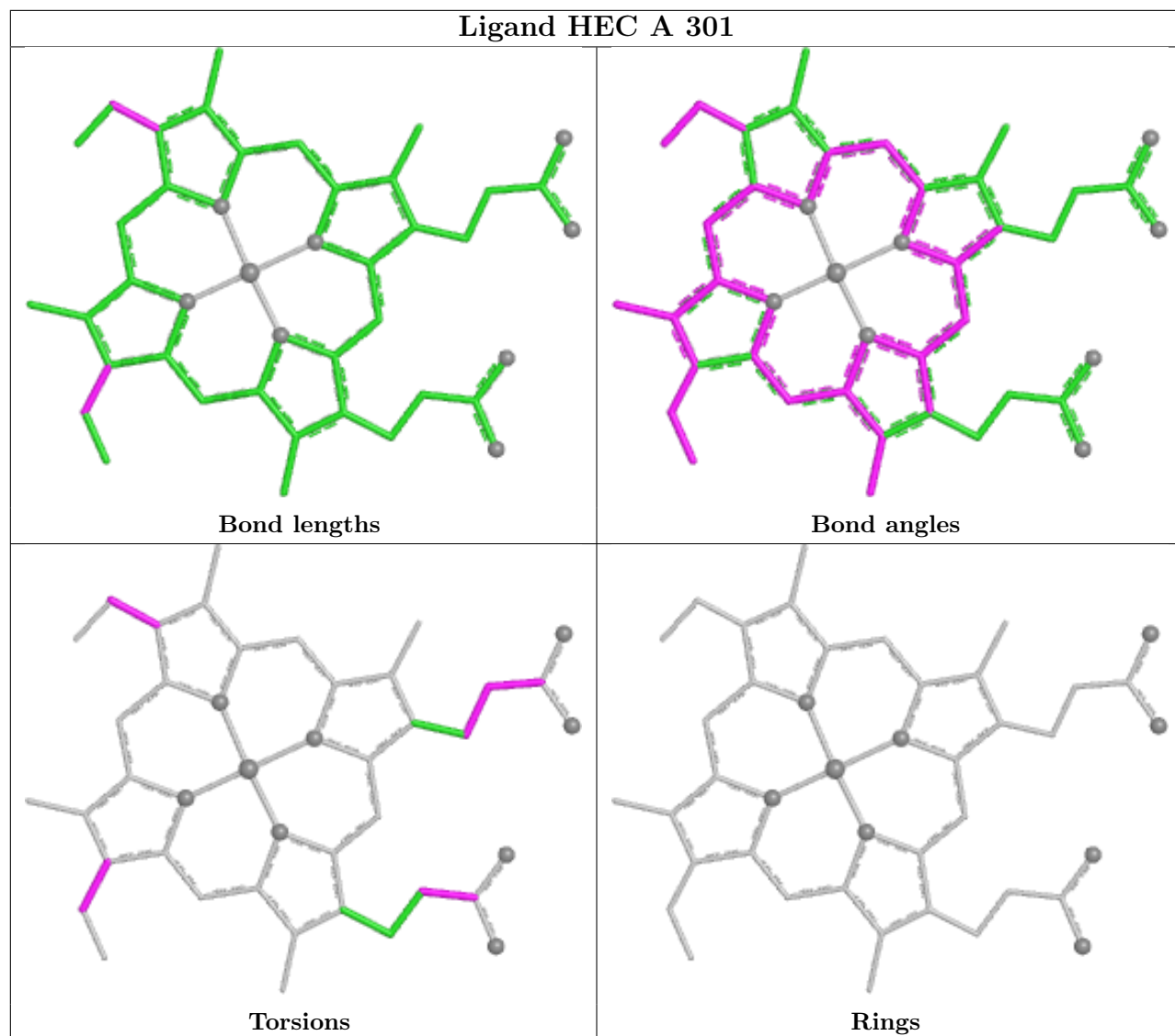




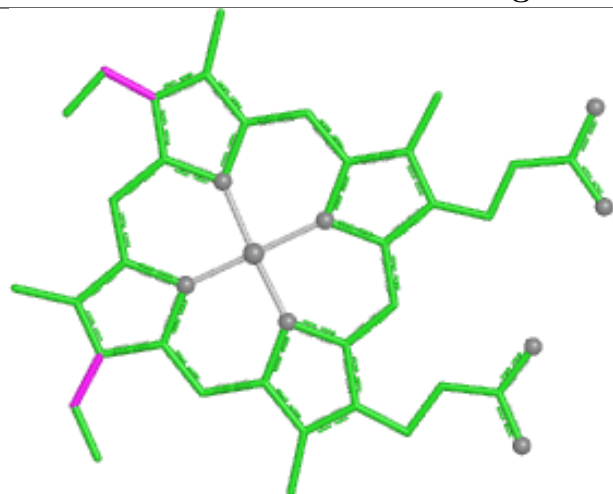




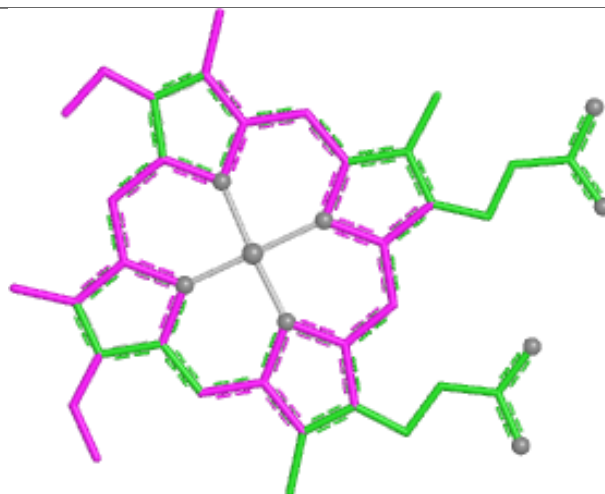




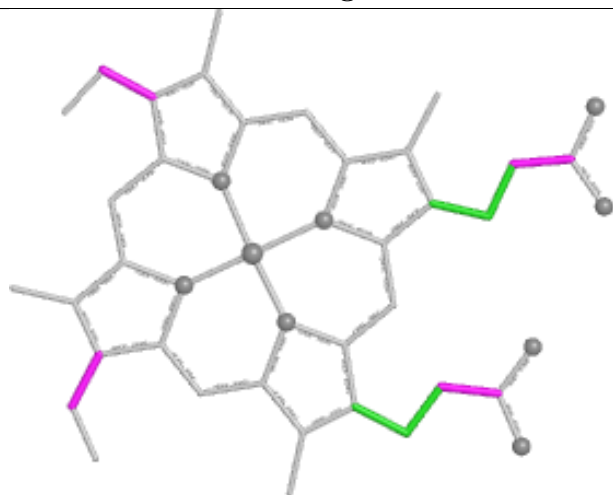
Ligand HEC A 294



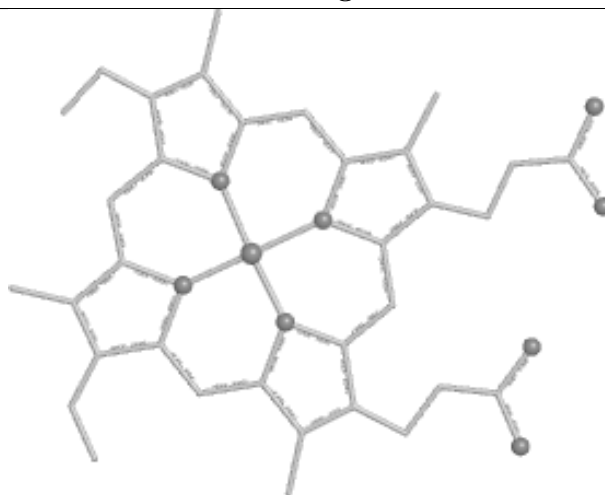
Bond lengths



Bond angles

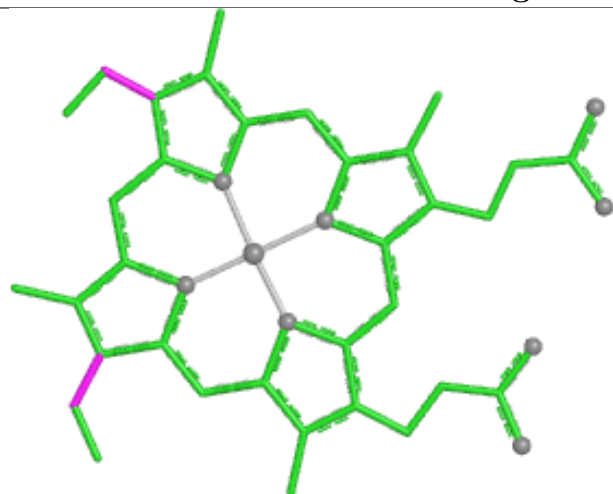


Torsions

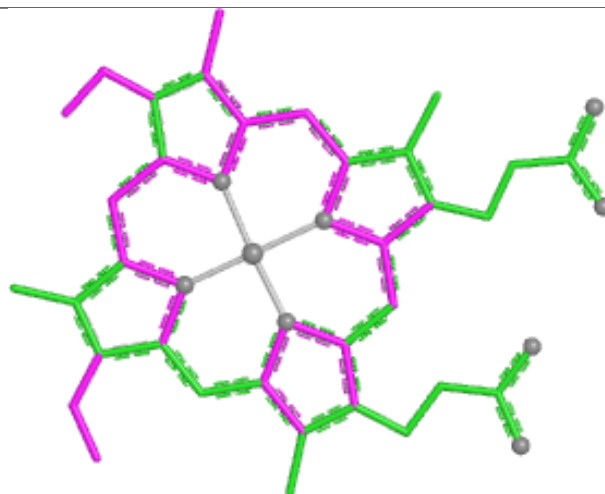


Rings

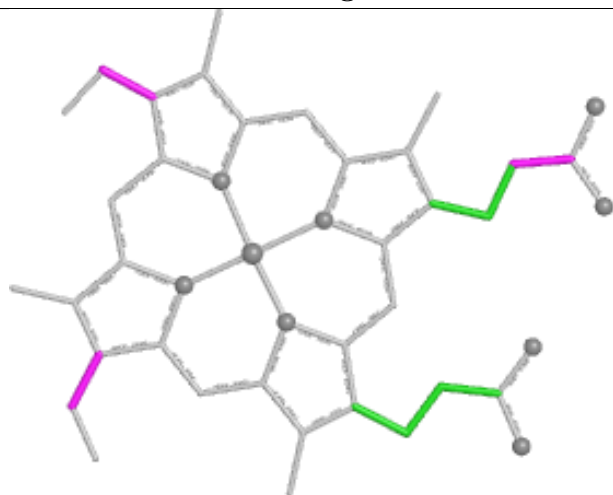
Ligand HEC A 298



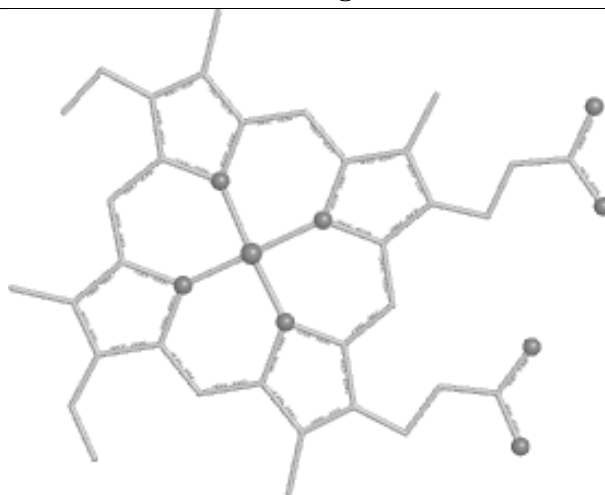
Bond lengths



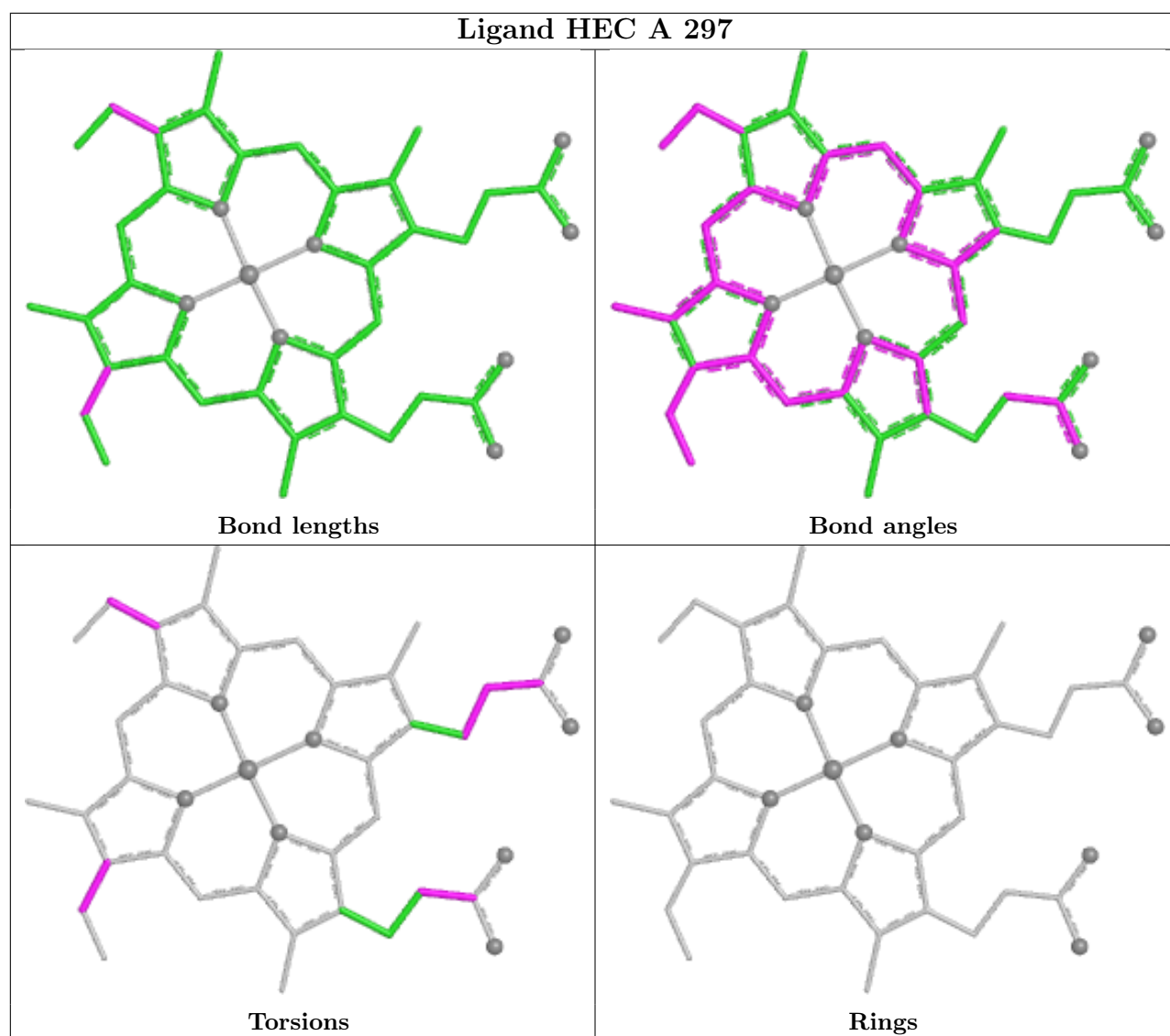
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/292 (98%)	0.21	16 (5%) 30 32	18, 27, 53, 93	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	7.1
1	A	254	PRO	6.5
1	A	252	ALA	4.0
1	A	292	PRO	3.8
1	A	255	ASN	3.5
1	A	250	ASP	3.5
1	A	45	ALA	2.8
1	A	251	PRO	2.8
1	A	291	ARG	2.7
1	A	84	ASN	2.7
1	A	249	ILE	2.6
1	A	174	ALA	2.2
1	A	168	PRO	2.2
1	A	167	LYS	2.1
1	A	121	LYS	2.0
1	A	166	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

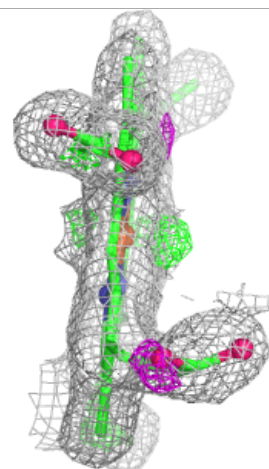
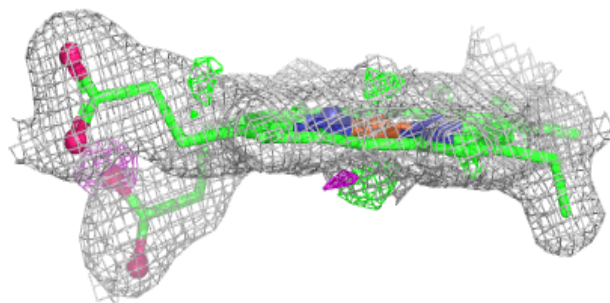
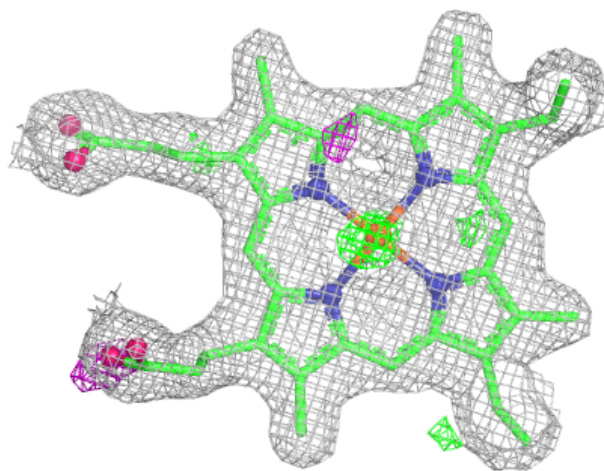
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	302	6/6	0.88	0.11	28,38,42,46	0
2	HEC	A	293	43/43	0.96	0.08	18,23,37,46	0
2	HEC	A	297	43/43	0.97	0.08	18,22,26,31	0
2	HEC	A	296	43/43	0.97	0.08	17,27,33,36	0
2	HEC	A	295	43/43	0.98	0.06	16,21,36,45	0
2	HEC	A	298	43/43	0.98	0.07	17,22,32,51	0
2	HEC	A	299	43/43	0.98	0.06	14,25,29,30	0
2	HEC	A	300	43/43	0.98	0.06	15,20,29,36	0
2	HEC	A	301	43/43	0.98	0.06	16,21,28,33	0
2	HEC	A	294	43/43	0.98	0.06	16,22,24,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

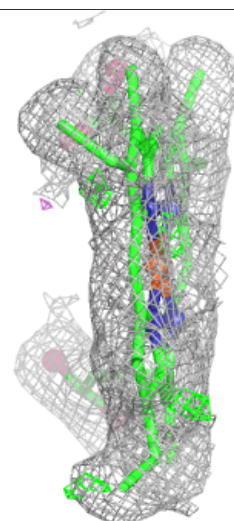
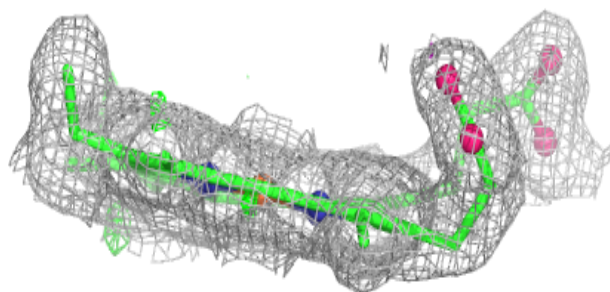
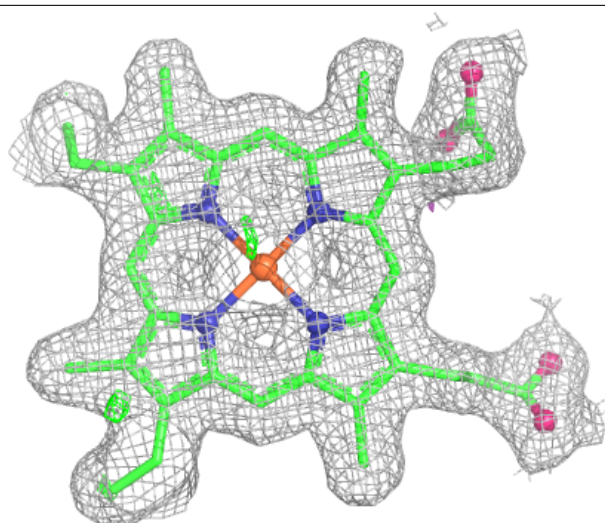
Electron density around HEC A 293:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



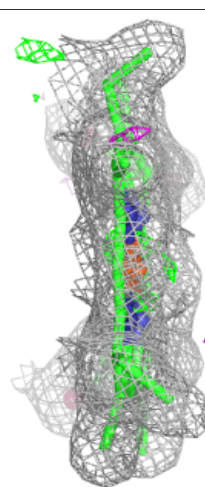
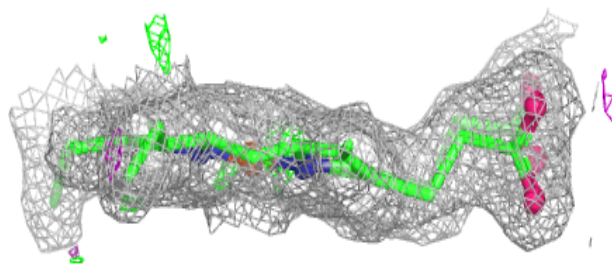
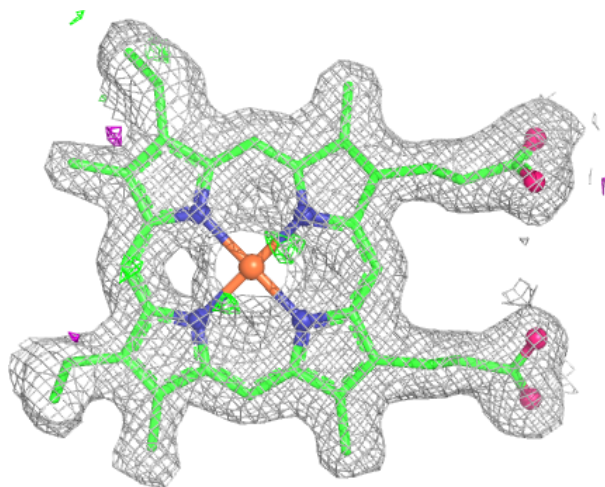
Electron density around HEC A 297:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



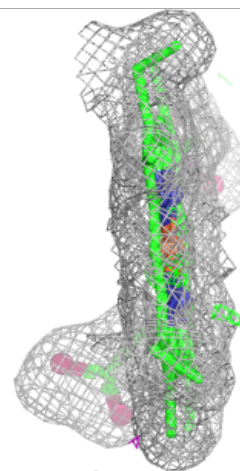
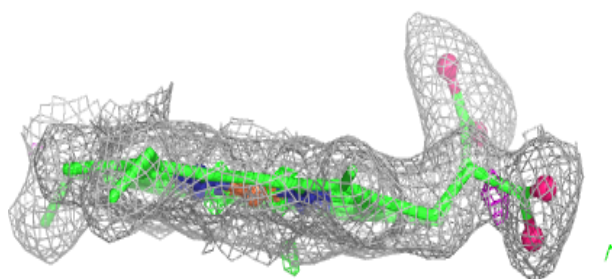
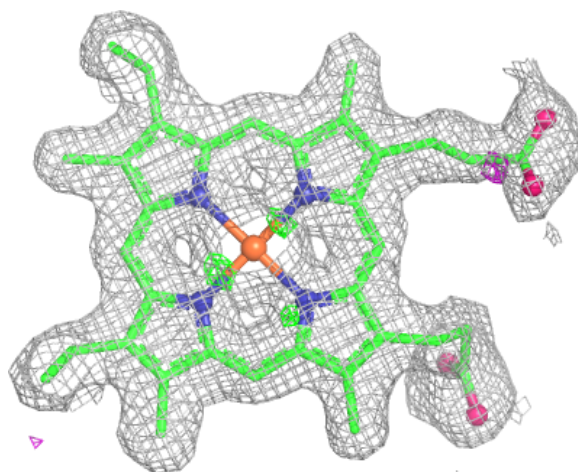
Electron density around HEC A 296:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



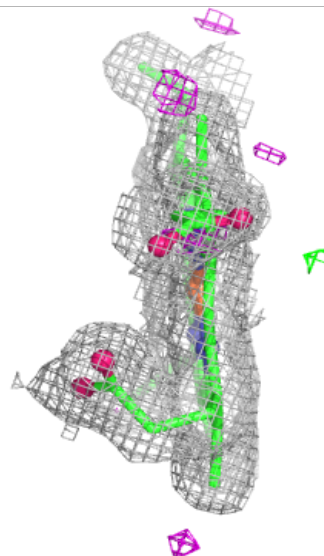
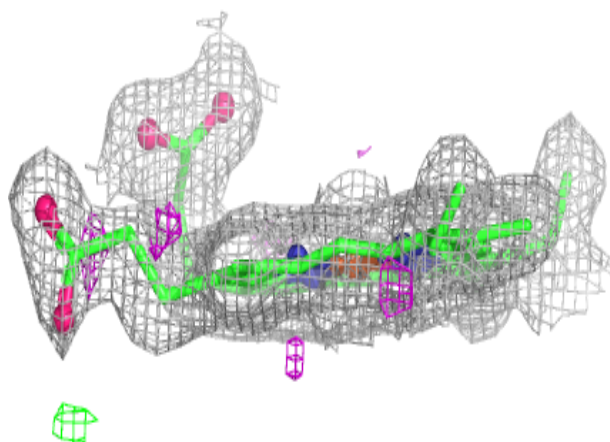
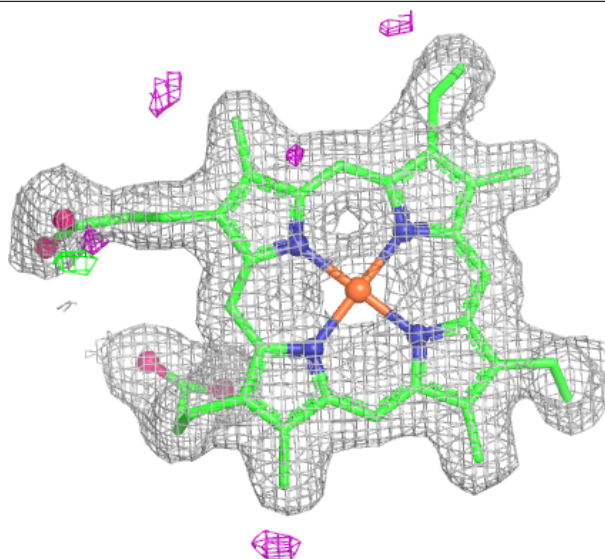
Electron density around HEC A 295:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



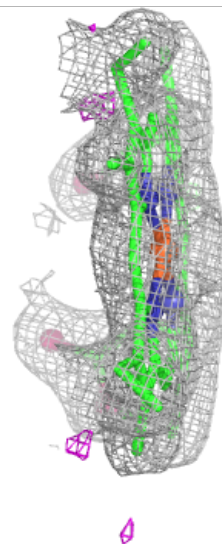
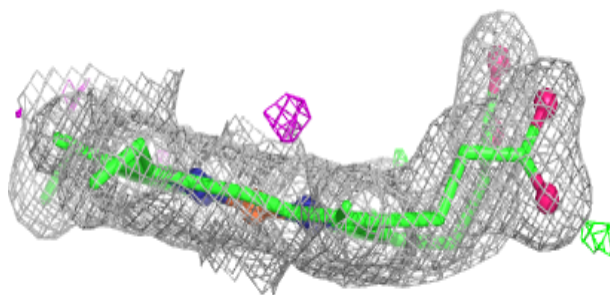
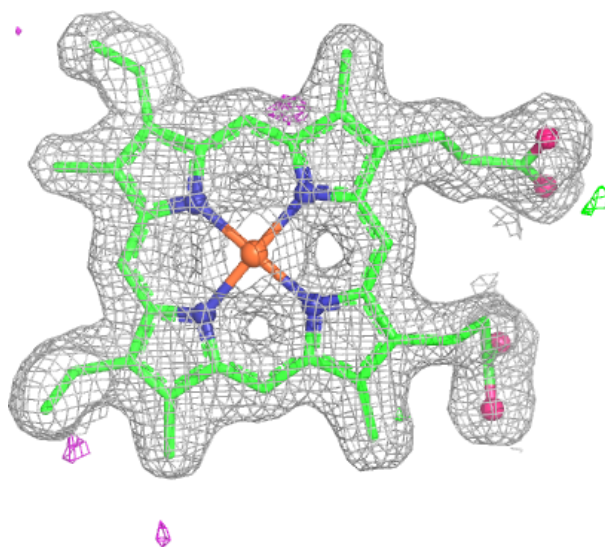
Electron density around HEC A 298:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



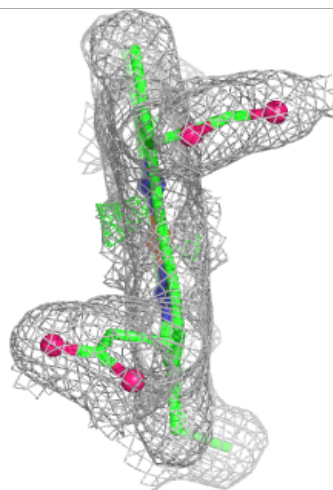
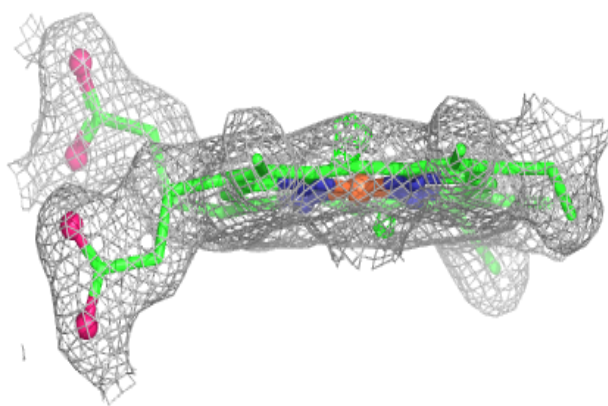
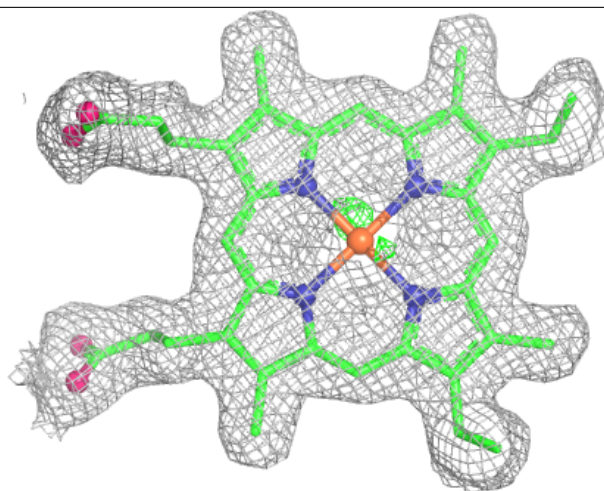
Electron density around HEC A 299:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



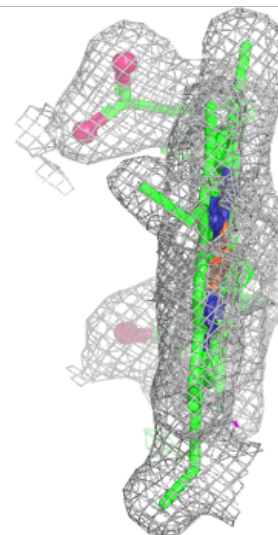
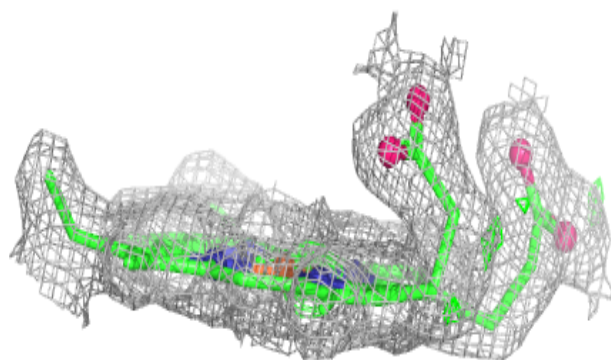
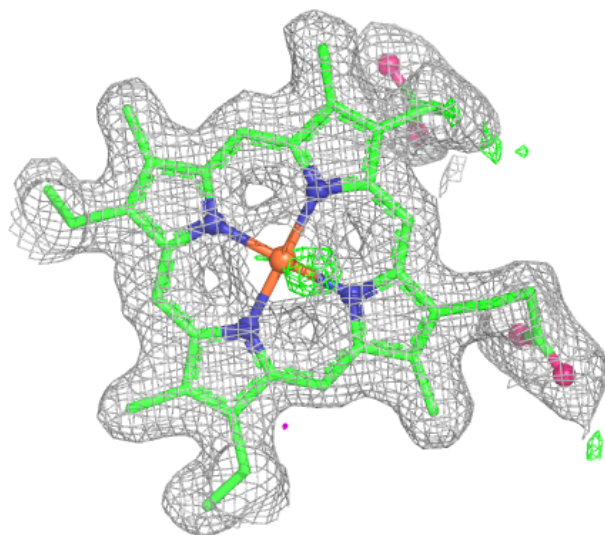
Electron density around HEC A 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



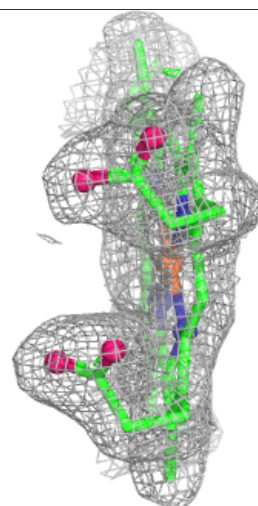
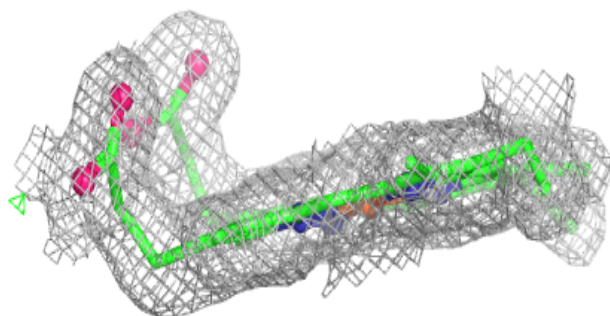
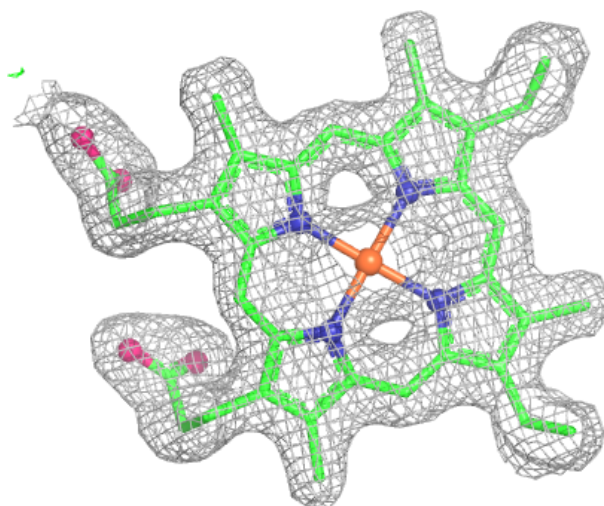
Electron density around HEC A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 294:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.